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Carrier scattering by impurity potentials with spatially variable dielectric functions

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A spatially dependent dielectric function $\epsilon(r)$ was introduced into the ionized-impurity potential in semiconductors, and the resultant scattering rates and mobilities were calculated. Without donor-acceptor compensation, only for very high doping would there be a marked deviation of the calculated mobility from the Brooks-Herring mobility. For compensated semiconductors, a compensation-ratio-dependent decrease is found in the calculated mobility. This decrease is found to be more pronounced the larger the electron effective mass of the semiconductor is. Available experimental data are discussed as a possible check of the proposed theory, and the need for new experiments is established.

I. INTRODUCTION

Scattering of electrons by ionized impurities has been described by Conwell and Weisskopf,[1] Dingle,[2] Brooks and Herring,[3,4] and many others. In their calculations of electron mobility they all use an impurity-ion potential $\phi_s(r)$ that includes the static dielectric constant of the material and an exponential screening factor (Yukawa potential)

$$\phi_s(r) = (Ze/4\pi\kappa\kappa_0 r)\exp(-r/R_0) , \quad (1)$$

where Ze is the charge of the ionized impurity, κ and κ_0 are the material and free-space dielectric constants, r is the radial distance from the impurity, and R_0 is the screening length. The exponential factor describes the electrostatic screening of the impurity-ion Coulomb potential by the mobile carriers that surround the ion and also by the fixed other ionized impurities. In the temperature regime where ionized impurity scattering is predominant, the mobility μ is given by the expression:

$$\mu = C_1 T^{3/2} N_I^{-1} B , \quad (2)$$

where T is the semiconductor temperature, N_I is the density of ionized impurities, C_1 is a constant incorporating the carrier effective mass and the static dielectric constant, and B is the screening factor that is given by

$$B = [\ln(1+\beta^2) - \beta^2/(1+\beta^2)] , \quad (3)$$

where

$$\beta = 2kR_0 \quad (4)$$

and k is the wave vector of the carriers and R_0 is the screening length.

Bound states of impurities in semiconductors have been, however, described by a wave-vector-dependent dielectric function $\epsilon(q)$.[5-8] The exact form of this $\epsilon(q)$ function is still under consideration and it seems desirable to seek new experimental information. Measurements of the electron scattering at ionized impurities offers a suitable experimental alternative to determine details of the impurity potential. In the usual treatment of Brooks-Herring and successors, as we have seen, however, the dielectric function is assumed to be constant.

Csavinszky[9] has calculated the impurity potential considering a spatially dependent dielectric function $\epsilon(r)$, where r is the radial distance from the impurity. The wave-vector-dependent dielectric function $\epsilon(q)$ can be obtained from a Fourier transform of the spatially dependent function $\epsilon(r)$. Csavinszky assumed an ideal case of an n-type semiconductor with no donor-acceptor compensation. Paesler[10] calculated the carrier mobility that results from scattering at ionized impurities with the Csavinszky potential working with the Brooks-Herring mathematical formalism. He predicted a sharp, concentration-dependent drop of the mobilities compared with the usual Brooks-Herring mobility. This prediction suffered from a mathematical error.[11] We performed the same calculations following also the Brooks-Herring formalism and we found no appreciable change in the mobility values for electron concentrations smaller than 10^{21} cm^{-3}. Richardson and Scarfone[12] report slightly different results.

Subsequently we also considered the effect of donor-acceptor compensation. At high compensations and low temperatures the carrier densities are very small and the screening is mainly due to the ionized impurities themselves.[13,14] We propose a scattering potential with a spatially dependent dielectric function $\epsilon(r)$, following Azuma,[15] and we recalculate the ionized-impurity limited mobility. The introduction of $\epsilon(r)$ in this case yields a lowering of the mobility compared with the mobility that is calculated using a scattering potential with a dielectric constant. This de-

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crease of the mobility depends on the compensation ratio of the impurities in the semiconductor and on its electron effective mass.

In Sec. II we discuss the case with no compensation. In Sec. III we report the results for the case of compensated semiconductors. In Sec. IV we discuss the experimental evidence that can be gathered from the data in the literature.

II. IDEAL CASE, NO COMPENSATION

In the following calculation, we use the Csavinszky potential, that is derived with the assumption of no compensation and electron density n equal to the ionized donor density N_{D+}. This potential is given by[9]

$$\phi_c = \frac{Ze}{4\pi\kappa\kappa_0 r}\left[C\exp\left(-\frac{r}{R_1}\right) + (1-C)\exp\left(-\frac{r}{R_2}\right)\right], \tag{5}$$

where C is a material parameter which depends on the electron concentration and R_1, R_2 are generalized screening lengths.[9] The Csavinszky potential is thus a linear combination of two Yukawa potentials.

The matrix element $H_{kk'}$ for scattering is given by the formula[16]

$$H_{kk'} = \int \psi_k^* e\phi_c(r)\psi_{k'}\, d^3r\ . \tag{6}$$

The scattering cross section $\sigma(\theta)$ can be calculated from the matrix element of scattering by means of the relation[16]

$$\sigma(\theta) = [(Vm/2\pi\hbar^2)|H_{k'k}|]^2\ , \tag{7}$$

where θ is the scattering angle, V is the crystal volume, m is the effective mass of the scattered carriers, $\hbar$ is Planck's constant divided by 2π. Knowing the scattering cross section we can calculate the momentum relaxation time τ_m which is given by the relation[16]

$$\tau_m^{-1} = \int_0^\pi \sigma(\theta)(1-\cos\theta)\sin\theta\, d\theta\ . \tag{8}$$

After performing the integration we obtain the result

$$\tau_m^{-1} \propto C^2\left[\ln(1+\beta_1^2) - \frac{\beta_1^2}{1+\beta_1^2}\right] + (1-C)^2\left[\ln(1+\beta_2^2) - \frac{\beta_2^2}{1+\beta_2^2}\right] + \frac{2C(1-C)}{\beta_2^2-\beta_1^2}\left[\beta_2^2\ln(1+\beta_1^2) - \beta_1^2\ln(1+\beta_2^2)\right] \equiv X, \tag{9}$$

where

$$\beta_1 = 2kR_1, \quad \beta_2 = 2kR_2\ . \tag{10}$$

The result in Eq. (9) differs from Paesler's result[10] in the third term; this error[11] caused the sharp drop of the mobilities in Paesler's paper.

The Brooks-Herring momentum relaxation time $\tau_{m\ \mathrm{BH}}$ is given by[16]

$$\tau_{m\ \mathrm{BH}}^{-1} \propto \ln(1+\beta_{\mathrm{BH}}^2) - \beta_{\mathrm{BH}}^2/(1+\beta_{\mathrm{BH}}^2) \equiv \psi\ , \tag{11}$$

where

$$\beta_{\mathrm{BH}}^2 = 2kR_0\ . \tag{12}$$

From Eqs. (11) and (9) we obtain

$$\mu/\mu_{\mathrm{BH}} = \psi/X\ , \tag{13}$$

where μ_{BH} is the Brooks-Herring mobility and μ is the new mobility which is calculated for the uncompensated case after the introduction of a spatially dependent dielectric function $\epsilon(r)$.

Figure 1 is a plot of the mobility ratio for Si, using the material parameters as given by Csavinszky for three different temperatures: 20, 77, and 300 K. We see immediately that the introduction of the spatially dependent dielectric function results in no appreciable change in the mobility for electron concentrations lower than 10^{21} cm^{-3}. This absence of an influence can be understood since the Brooks-Herring scattering potential and the Csavinszky scattering potential do not differ appreciably in this density region as can be seen in Fig. 2. This is due to the self-consistency of the Csavinszky treatment which reduces the effect of the spatial dependence of the dielectric function by shifting electron charge into regions surrounding the impurity where the dielectric function is much smaller than the dielectric constant. For high electron densities the two scattering potentials are no longer the same (Fig. 2) and the characteristic length of their difference can be compared with the very small screening lengths. For very high electron densities ($n > 10^{21}$ cm^{-3}), the mobilities ratio becomes temperature

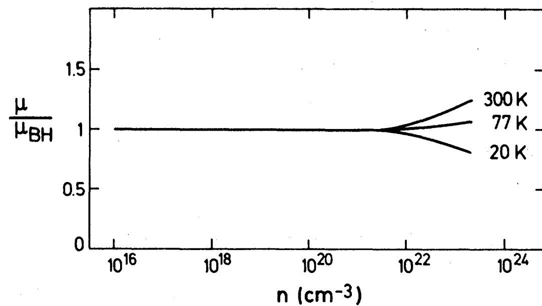

FIG. 1. Ratio of the mobility μ calculated with a spatially dependent dielectric function to the Brooks-Herring mobility μ_{BH} vs the carrier concentration n for uncompensated Si, at 20, 77, and 300 K.

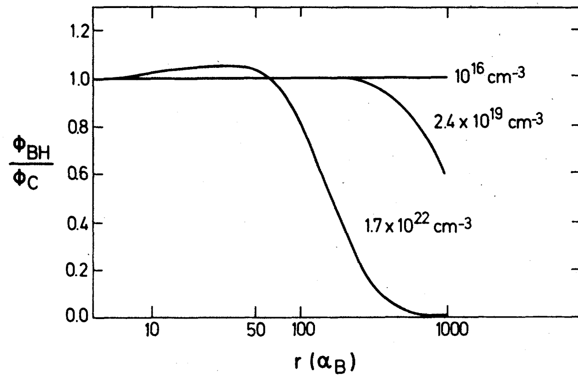

FIG. 2. Ratio of the Brooks-Herring potential ϕ_{BH} to the Csavinszky potential ϕ_C vs the distance r from the impurity for three difference carrier concentrations n. α_B is the Bohr radius.

dependent because an elevation of the temperature raises the kinetic energy of the electrons; carriers with increased kinetic energy penetrate more deeply into the impurity potential, i.e., closer to the impurity ion. In these closer regions, the Csavinszky potential does deviate from the Brooks-Herring potential depending upon the distance r from the impurity ion (Fig. 2). Consequently the mobility deviates accordingly from the Brooks-Herring mobility.

The main result for uncompensated semiconductors is that the introduction of the variable dielectric function does not have a pronounced effect on the scattering by ionized impurities and consequently on the mobility. The densities at which an effect does exist are so high that we can no longer consider the material to be a semiconductor.

III. REAL CASE, IMPURITY COMPENSATION

The screening of ionized impurities in compensated semiconductors has been investigated by Cuevas,[13,14] Falicov,[14] Stern[17] and others. The main feature in this case is that the compensation appreciably reduces the number of free electrons in the crystal, especially at low temperatures, while keeping a large number of scattering centers. The concentration N_I of ionized impurities equals 2 times the concentration of the minority impurities. Thus in the case of n-type material the minority impurities are negatively charged acceptors and we have

$$N_I = 2N_{A^-} , \tag{14}$$

where N_{A^-} is the concentration of the acceptors. All of the acceptors are ionized and the concentration of ionized donors N_{D^+} equals the concentration of the ionized acceptors.

The screening is now mainly a result of the ionized impurities themselves. The screening of ionized impurities by other ionized impurities was predicted also by Brooks; Cuevas and Falicov were the first who made systematic measurements and presented a theory to prove it. An important result of their calculation and experiment is that the lowering of compensation (introduction of more majority impurities that remain neutral) improves the screening so that the screening length is reduced. Thus, at higher concentrations of majority impurities it is possible to obtain larger mobilities.[14] The correlation theory of Falicov and Cuevas explains this screening improvement.[14] The introduction of more majority impurities increases the probability of the formation of ionized donor-acceptors pairs, so that the screening between them is improved. The total concentration of ionized impurities does not change because it equals 2 times the concentration of the minority impurities (13) and does not depend on the concentration of the majority impurities.

Scattering occurs only in regions fairly close to the ionized impurities, where the variable dielectric function differs appreciably from the static dielectric constant.

The screening length R_0 in the Falicov and Cuevas correlation theory is given by the relation

$$R_0 = [2\pi^{1/3}(N_D - N_A)^{1/3}]^{-1} , \tag{15}$$

where N_D is the donor concentration and N_A is the acceptor concentration. It differs a little from the screening lengths that are calculated by Stern,[17] for temperatures approaching absolute zero.

In order to calculate the change of mobility after introducing the spatial variation of the dielectric function in the case of compensation, we propose an ionized impurity potential following Azuma.[15] This potential is derived by multiplying the screened Coulomb potential with the inverse of the spatially dependent dielectric function, and is justified by the lack of many free carriers which would make necessary the self-consistent Csavinszky calculation. The proposed potential is given by the relation

$$\phi_v(r) = \left[\frac{Ze}{4\pi\kappa_0 r} \exp\left(-\frac{r}{R_0}\right)\right] \times \left[\frac{1}{\epsilon_0} + A\exp(-\alpha r) + (1-A)\exp(-\beta r) - \frac{1}{\epsilon_0}\exp(-\gamma r)\right] . \tag{16}$$

The first bracketed term is the screened Coulomb potential, where R_0 is the screening length, and the second set of brackets is the inverse spatially dependent dielectric function as proposed by Wal-

ter and Cohen,[18] Bernholc and Pantelides,[7] and others. ϵ_0 is the static dielectric constant and A, α, β, γ are material parameters given by several authors.[7,18]

Using the potential of Eq. (16) we perform the calculation of the mobilities ratio in the same way as in Sec. I. Thus we obtain first the matrix element of scattering [Eq. (6)], then the scattering cross section [Eq. (7)], and finally the momentum relaxation time [Eq. (8)]. The final result for the ratio of mobilities is

$$\frac{\mu}{\mu_s}=\frac{\psi}{\Lambda}, \tag{17}$$

where

$$\psi=\ln[1+(2kR_0)^2]-\frac{(2kR_0)^2}{1+(2kR_0)^2} \tag{18}$$

and

$$\begin{aligned}
\Lambda=&\frac{1}{\epsilon_0^2}\left[\ln(1+(2kR_0)^2]-\frac{(2kR_0)^2}{1+(2kR_0)^2}\right]+A^2\left\{\ln\left[1+\left(\frac{2k}{\alpha}\right)^2\right]-\frac{(2k/\alpha)^2}{1+(2k/\alpha)^2}\right\}\\
&+(1-A)^2\left\{\ln\left[1+\left(\frac{2k}{\beta}\right)^2\right]-\frac{(2k/\beta)^2}{1+(2k/\beta)^2}\right\}+\frac{1}{\epsilon_0^2}\left\{\ln\left[1+\left(\frac{2k}{\gamma}\right)^2\right]-\frac{(2k/\gamma)^2}{1+(2k/\gamma)^2}\right\}\\
&+\frac{2A}{\epsilon_0}\left(\frac{1}{(2k/\alpha)^2-(2kR_0)^2}\right)\left\{\left(\frac{2k}{\alpha}\right)^2\ln[1+(2kR_0)^2]-(2kR_0)^2\ln\left[1+\left(\frac{2k}{\alpha}\right)^2\right]\right\}\\
&+\frac{2(1-A)}{\epsilon_0}\left(\frac{1}{(2k/\beta)^2-(2kR_0)^2}\right)\left\{\left(\frac{2k}{\beta}\right)^2\ln[1+(2kR_0)^2]-(2kR_0)^2\ln\left[1+\left(\frac{2k}{\beta}\right)^2\right]\right\}\\
&-\frac{2}{\epsilon_0^2}\left[\frac{1}{(2k/\gamma)^2-(2kR_0)^2}\right]\left\{\left(\frac{2k}{\gamma}\right)^2\ln[1+(2kR_0)^2]-(2kR_0)^2\ln\left[1+\left(\frac{2k}{\gamma}\right)^2\right]\right\}\\
&+2A(1-A)\left(\frac{1}{(2k/\beta)^2-(2k/\alpha)^2}\right)\left\{\left(\frac{2k}{\beta}\right)^2\ln\left[1+\left(\frac{2k}{\alpha}\right)^2\right]-\left(\frac{2k}{\alpha}\right)^2\ln\left[1+\left(\frac{2k}{\beta}\right)^2\right]\right\}\\
&-\frac{2A}{\epsilon_0}\left(\frac{1}{(2k/\gamma)^2-(2k/\alpha)^2}\right)\left\{\left(\frac{2k}{\gamma}\right)^2\ln\left[1+\left(\frac{2k}{\alpha}\right)^2\right]-\left(\frac{2k}{\alpha}\right)^2\ln\left[1+\left(\frac{2k}{\gamma}\right)^2\right]\right\}\\
&-\frac{2(1-A)}{\epsilon_0}\left(\frac{1}{(2k/\gamma)^2-(2k/\beta)^2}\right)\left\{\left(\frac{2k}{\gamma}\right)^2\ln\left[1+\left(\frac{2k}{\beta}\right)^2\right]-\left(\frac{2k}{\beta^2}\right)^2\ln\left[1+\left(\frac{2k}{\gamma}\right)^2\right]\right\}.
\end{aligned} \tag{19}$$

Figure 3 is a plot of the mobilities ratio μ/μ_s as a function of the screening length R_0, for GaAs, Si, and GaP, for three temperatures and with the material parameters A, α, β, γ given in Table I. As the screening length becomes shorter the mobilities ratio μ/μ_s decreases and the influence of the variable dielectric function on the mobility value becomes more pronounced. This effect is strong for GaP, less for Si, and almost insignificant for GaAs; it becomes more pronounced the larger the temperature is. The differences among the several materials arise from the different effective electron masses. The kinetic energy of the electrons is proportional to their effective mass and the temperature. Electrons with increased kinetic energy penetrate deeper into the impurity potential where the spatially dependent dielectric function differs more from the static dielectric constant. GaAs has a lower effective electron mass than Si and GaP and for this reason the mobilities ratio for GaAs is close to 1. Also similar is the role of the temperature. Thus at elevated temperatures the kinetic energy of the scattered electrons is higher and the mobilities ratio is

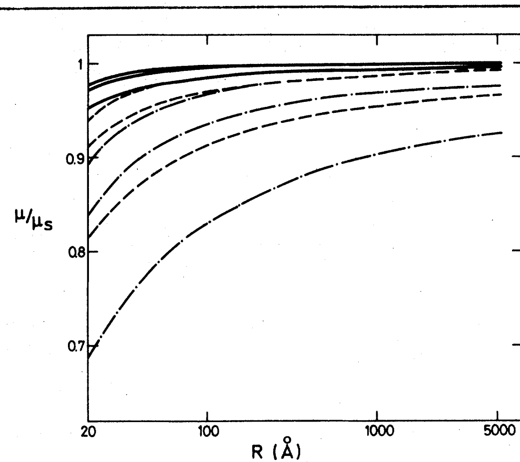

FIG. 3. Ratio of the mobility μ calculated with a spatially dependent dielectric function to the mobility μ_s calculated with a dielectric constant vs the screening length R for compensated GaAs (full lines), Si (dashed lines), and GaP (dashed-dotted lines) at three temperatures (30, 77, and 300 K). For each material the uppermost curve is plotted for 30 K, the middle curve for 77 K, and the lowest curve for 300 K. (It must be mentioned that at 300 K some of our assumptions are not valid but the 330-K curve elucidates the effect of temperature elevation.)

TABLE I. Material parameters for GaAs, Si, and GaP. (The parameters were taken from Ref. 7.)

	A	α (a.u.)	β (a.u.)	γ (a.u.)
GaAs	1.105	0.717	0.292	0.390
Si	1.104	0.710	0.288	2.645
GaP	1.144	0.855	0.448	2.643

lower, than at lower temperatures.

The screening length as a function of the compensation ratio for a given donor concentration can be calculated from Eq. (15). The mobilities ratio as a function of compensation ratio for a given donor or acceptor concentration can be subsequently calculated. The results for some typical values of donor concentrations for GaAs, Si, and GaP are plotted in Figs. 4, 5, and 6 for three temperatures.

The mobilities ratio is always smaller than 1. This means that the introduction of the spatially dependent dielectric function lowers the calculated mobility. The mobility becomes smaller as the screening length gets shorter because the electrons are scattered near the impurity where there is the largest difference between the variable dielectric function and the static dielectric constant. Thus the calculated mobility becomes smaller at lower compensations because then the screening length is shorter. This lowering of the mobility implies a stronger scattering potential and is in agreement with Bernholc and Pantelides,[7] who report that the use of a variable dielectric function increases the binding energy of the impurity.

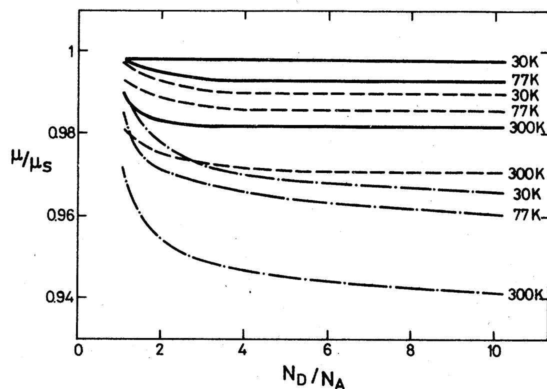

FIG. 4. Ratio of the mobility μ calculated with a variable dielectric function to the mobility μ_S calculated with a dielectric constant vs the compensation ratio N_D/N_A for GaAs at three different temperatures (30, 77, and 300 K) for three different donor concentrations: 10^{17} cm^{-3} (full lines), 10^{18} cm^{-3} (dashed lines), and 10^{19} cm^{-3} (dashed-dotted lines).

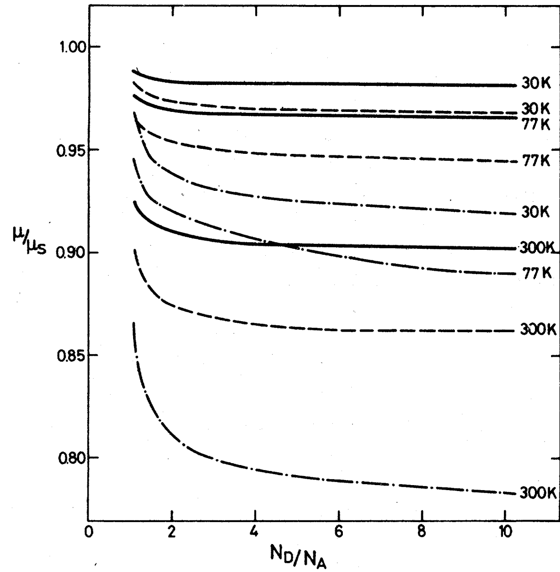

FIG. 5. Same as Fig. 4, for Si.

IV. DISCUSSION AND COMPARISON WITH EXPERIMENTAL DATA

The above results strongly suggest that the introduction of a spatially dependent dielectric function, in place of the static dielectric constant, into

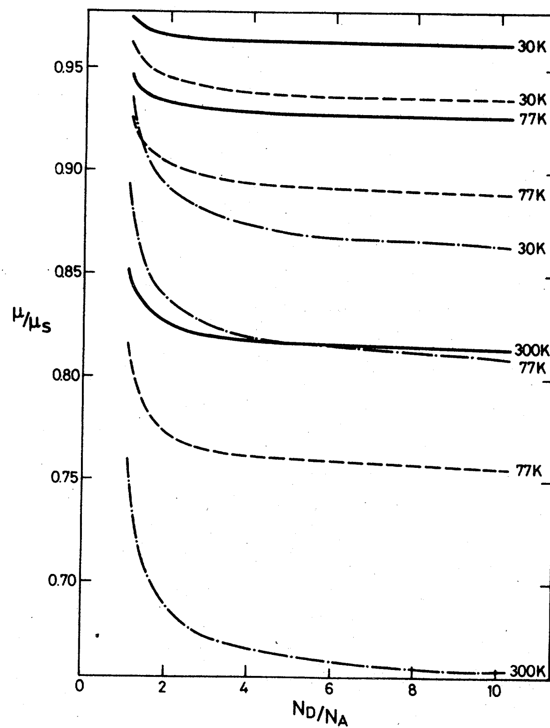

FIG. 6. Same as Fig. 4, for GaP.

the scattering potential lowers the calculated mobility. This effect is almost nonexistent for the idealized case of no donor-acceptor compensation but it is important in the real case of compensated semiconductors. This mobility reduction should be evident in the comparison of carefully measured mobilities with the calculated mobilities with and without a variable dielectric function. This comparison could in principle also help to choose among the proposed dielectric functions by several authors.

We scanned the literature data for mobility measurements trying to find evidence for a discrepancy between experimental mobilities and mobilities calculated with a static dielectric constant. The experimental values should be lower than the theoretical values. But the evaluation of the experimental data is complicated since most authors use several adjustable parameters in order to fit their experimental results to the theory. These parameters are the effective electron mass, the activation energy, and the concentration and compensation of the impurities in the used samples. The calculated mobility depends strongly on these parameters and any uncertainty in them influences the mobility. Thus any possible small disagreement between theory and experiment may be hidden in the deviation of the calculated mobility due to the error in the values of these parameters. Although there are now established values for the effective electron mass and activation energy for the most important semiconductors, the concentration and the compensation of the impurities must be measured in any experiment. This measurement is difficult. An additional difficulty is that it is almost impossible to obtain crystals with entirely homogeneous doping. Electrical measurements of compensation can give different results from optical measurements as has been shown by Kamiya and Wagner.[19] Thus the error in the calculated mobility due to the error in the measurement of the donor and acceptor concentration and the deviation of homogeneity can be probably as large as the difference between the mobilities calculated with and without a spatially dependent dielectric function.

Proper superposition of lattice and ionized-impurity scattering presents a further difficulty. Addition of reciprocal mobility contributions is a poor approximation. An improvement consists in using a "mixed-scattering" formula, as explained by Debye and Conwell.[20] Tests of theories for impurity scattering are thus particularly difficult at temperatures high enough to cause substantial lattice scattering.

Long and Myers[21] have done careful measurements of the mobility in the regime of ionized impurity scattering with Si crystals. They admit that there is an appreciable error in the measurement of donor and acceptor concentrations but they also find that the Brooks-Herring theory overestimates the mobility. Norton and Levinstein[22] have made a mobility analysis of Ge and they found good agreement with the Brooks-Herring theory but they fit the data with three adjustable parameters. Brown and Bray[23] also find that the Brooks-Herring theory overestimates the mobility in Ge by as much as 50% for high impurity concentrations. In a recent summary concerning Si, Li[24] noted the overestimation by the Brooks-Herring theory and suggested electron-electron scattering and scattering anisotropy to account for the lower experimental mobilities. Wolfe, Stillman, and Lindley[25] find good agreement between theory and experiment in high-purity GaAs. Rode[26] reports that the Brooks-Herring theory overestimates slightly the mobility in GaAs. The experimental data for ionized-impurity scattering in GaP are not yet conclusive but Rode[27] suggests that the calculated mobility in GaP is probably higher than the experimental.

Ralph, Simpson, and Elliott[28] (RSE) have also treated the problem of the details of the scattering potential near an ionized impurity. They discuss the frequent observation that the theoretical mobility tends to exceed the experimental one; they further stress the fact that the mobility appears to depend on the chemical identity of the dopant. Central-cell corrections are proposed to reduce these discrepancies. RSE use the "chemical shift" (difference between the hydrogenic binding energy and the observed energy) as an additional scattering potential which depends upon the chemical nature of the impurity and is assumed to be a δ function at the ion site. The ionized-impurity scattering potential is thus composed of the conventional screened Coulomb long-range part plus the short-range "chemical shift". Any space dependence of the dielectric function is not taken account. A detailed critical discussion of the present status concerning treatments of the "chemical shift" has recently been given by Pantelides.[29] He points out the shortcomings of assuming a potential derived from the "chemical shift" and stresses the need for considering intervalley effects and for introducing a variable dielectric function.

Both approaches (RSE's and ours) reduce the value of the calculated mobilities resulting from scattering at ionized impurities compared to the original Brooks-Herring treatment. RSE find, for example, a mobility reduction of about 20% in Si with 10^{18} cm^{-3} doping at 300 K (see Fig. 2 of Ref. 28). Different chemical impurities produce variations of mobilities up to 10%. We find for

Si with 10^{18} cm^{-3} donor concentration, 10% compensation, at 300 K a mobility reduction of about 15% (Fig. 5). We have neglected the chemical nature of the impurity, which might, however, indirectly influence actual compensation during crystal preparation.

We feel that the spatially dependent dielectric function plays a role in the discrepancies between experiment and theory. The use of a spatially independent dielectric constant is a crude approximation near the impurity and may be the cause of the overestimation of the theoretical mobility that is reported by many authors.

We are currently preparing experiments to accurately measure the concentration- and compensation-dependent mobility.

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